Employing Sensitivity Derivatives to Estimate Uncertainty Propagation in CFD

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Abstract

Two methods that exploit the availability of sensitivity derivatives are successfully employed to predict uncertainty propagation through Computational Fluid Dynamics (CFD) code for an inviscid airfoil problem. An approximate statistical second-moment method and a Sensitivity Derivative Enhanced Monte Carlo (SDEMC) method are successfully demonstrated on a two-dimensional model problem. First- and second-order sensitivity derivatives of code output with respect to code input are obtained through an efficient incremental iterative approach. Given uncertainties in statistically independent, random, normally distributed flow parameters (input variables); these sensitivity derivatives enable one to formulate first- and second-order Taylor Series approximations for the mean and variance of CFD output quantities. Additionally, incorporation of the first-order sensitivity derivatives into the data reduction phase of a conventional Monte Carlo (MC) simulation allows for improved accuracy in determining the first moment of the CFD output. Both methods are compared to results generated using a conventional MC method. The methods that exploit the availability of sensitivity derivatives are found to be valid when considering small deviations from input mean values.

Introduction

In Computational Fluid Dynamics (CFD), the computation of sensitivity derivatives (SD) of CFD code output, with respect to code input parameters, affords information which can be used to estimate uncertainty propagation; that is, the extent to which the function output is affected by uncertainties in input parameters. In [1] it is shown that a statistical First-Order Second Moment (FOSM) method and Automatic Differentiation (AD) can be used to efficiently propagate input uncertainties through finite element analyses to approximate output uncertainty. In the present study, this FOSM method, as well as a Second-Order Second Moment (SOSM) method is demonstrated. The results of the FOSM and SOSM approximate methods are compared to results obtained using traditional MC techniques. Additionally, the availability of CFD SD may be incorporated into variance reduction schemes for traditional MC simulations. The strategy of exploiting the availability of SD for improved sampling was proposed in [2]. This proposed methodology for variance reduction, Sensitivity Derivative-Enhanced Sampling (SDES), is demonstrated herein on a CFD code.

For the present study, we assume that the input uncertainty quantification is given by independent normally distributed random variables. Although the strategy presented herein is also applicable to correlated and/or non-normally distributed variables, the analysis and resulting equations become more complex. We also assume that sources of uncertainty are exclusively those due to code input parameters, i.e., due to sources external to the CFD code simulation. We address the assessment of everyday operational fluctuations on performance loss, not catastrophe. Consequently, we are most concerned with behavior due to probable fluctuations, i.e., near the mean of probability density function (pdf).

Uncertainty Propagation

In the present study the input random variables are designated as $\mathbf{b}=\{b_1,\ldots,b_n\}$, with mean values, $\overline{\mathbf{b}}=\{\overline{b}_1,\ldots,\overline{b}_n\}$, and standard deviations $\sigma_{\mathbf{b}}=\{\sigma_{b_1},\ldots,\sigma_{b_n}\}$. The CFD output function, **F= F(b),** is a function of the input random variables, **b.**

Traditional Monte Carlo Method

The most straightforward way to compute the expected value of **F(b)**, designated as $\overline{\mathbf{F}}(\mathbf{b})$, and the variance, designated as $\sigma_{\mathbf{F}}{}^2$ is to employ a traditional MC analysis and calculate the mean and variance as

$$\overline{\mathbf{F}}(\mathrm{b})=\frac{1}{N}\sum_{i=1}^{N}\mathbf{F}(\mathrm{b_i}) \qquad \sigma_F^2=\frac{\sum_{i=1}^{N}(\mathbf{F}(\mathrm{b_i})-\overline{\mathbf{F}}(\mathrm{b}))^2}{N-1} \quad (1).$$

The problem with a traditional MC simulation is that in order to get an accurate prediction of the output mean and variance one may have to perform thousands of runs which is often not feasible with high fidelity CFD codes.

Sensitivity Derivative Enhanced Monte Carlo Method (SDEMC)

One naturally looks for ways to improve the convergence of the traditional MC method. In [2] the availability of the SD is exploited to achieve variance reduction via SDES techniques. SDES applied to a traditional MC is termed herein as the Sensitivity Derivative Enhanced Monte Carlo (SDEMC) method. The SDEMC method employs the calculation of a first-order Taylor series approximation, $\mathbf{F}_1(\mathbf{b})$ expanded about the mean values of the input parameters $\overline{\mathbf{b}}$ as

$$\mathbf{F}_1(\mathbf{b})=\mathbf{F}(\overline{\mathbf{b}})+\sum_{i=1}^{n}\frac{\partial\mathbf{F}}{\partial \mathrm{b_i}}(\mathrm{b_i}-\overline{\mathrm{b}}_\mathrm{i}) \quad (2).$$

Further analysis (shown in [2]) suggests that by incorporating knowledge of the SD evaluated at the input parameter mean values, one can approximate $\overline{\mathbf{F}}(\mathbf{b})$ by applying a MC simulation to $\mathbf{F}_1(\mathbf{b})$. The resulting SDEMC approximation for the mean of the output function, **F** is given as

$$\overline{\mathbf{F}}(\mathbf{b})\approx\mathbf{F}(\overline{\mathbf{b}})+\frac{1}{N}\sum_{i=1}^{n}\sum_{j=1}^{N}\frac{\partial\mathbf{F}}{\partial \mathrm{b_i}}(\mathrm{b_{i,j}}-\overline{\mathrm{b}}_\mathrm{i}) \quad (3)$$

Approximate Statistical Moment Method

The approximate statistical moments are calculated for the first moment (expected value) and second moment (variance) applying standard procedures to either first- or second-order Taylor series approximations of the output function of interest where derivatives are evaluated at the mean values, $\bar{\mathbf{b}}$. The Taylor series approximations are

$$\text{FO:} \qquad \mathbf{F}(\mathbf{b}) = \mathbf{F}(\bar{\mathbf{b}}) + \sum_{i=1}^{n} \frac{\partial \mathbf{F}}{\partial b_i}(b_i - \bar{b}_i) \quad (4)$$

$$\text{SO:} \qquad \mathbf{F}(\mathbf{b}) = \mathbf{F}(\bar{\mathbf{b}}) + \sum_{i=1}^{n} \frac{\partial \mathbf{F}}{\partial b_i}(b_i - \bar{b}_i) + \frac{1}{2}\sum_{j=1}^{n}\sum_{i=1}^{n} \frac{\partial^2 \mathbf{F}}{\partial b_i \partial b_j}(b_i - \bar{b}_i)(b_j - \bar{b}_j) \quad (5)$$

For normally distributed input variables, one then obtains the following approximations for the mean and variance of the output function, **F:**

$$\text{FO:} \qquad \bar{\mathbf{F}} = \mathbf{F}(\bar{\mathbf{b}}) \qquad\qquad \sigma_{\mathbf{F}}^{\,2} = \sum_{i=1}^{n}\left(\frac{\partial \mathbf{F}}{\partial b_i}\sigma_{b_i}\right)^2 \quad (6)$$

$$\text{SO:} \quad \bar{\mathbf{F}} = \mathbf{F}(\bar{\mathbf{b}}) + \frac{1}{2!}\sum_{i=1}^{n}\frac{\partial^2 \mathbf{F}}{\partial b_i^{\,2}}\sigma_{b_i}^{\,2} \qquad \sigma_{\mathbf{F}}^{\,2} = \sum_{i=1}^{n}\left(\frac{\partial \mathbf{F}}{\partial b_i}\sigma_{b_i}\right)^2 + \frac{1}{2!}\sum_{j=1}^{n}\sum_{i=1}^{n}\left(\frac{\partial^2 \mathbf{F}}{\partial b_i \partial b_j}\sigma_{b_i}\sigma_{b_j}\right)^2 \quad (7)$$

where derivatives are evaluated at the mean values, $\bar{\mathbf{b}}$. Note in Eq. (7) that the second-order mean output, $\bar{\mathbf{F}}$, is not at the mean values of input $\bar{\mathbf{b}}$, i.e., $\bar{\mathbf{F}} \neq \mathbf{F}(\bar{\mathbf{b}})$. Equations (6) represent a FO method and Eq. (7) a SO method for examining uncertainty propagation. The methods are straightforward with the difficulty largely lying in computation of the SD. The very efficient method used here to obtain such derivatives is presented in [3.]

Application to 2-D Euler CFD

An initial investigation of uncertainty propagation in CFD using both a first and second-order approximate statistical moment method was done for several quasi 1-D problems using Euler Code [4]. This methodology as well as the SDEMC methodology is demonstrated herein for a 2-D inviscid steady subsonic flow over a NACA 64A410 airfoil using an Euler code [3]. A 129 x 33 C-mesh computational grid is used. For the current study, the airfoil angle of attack, α and the free-stream Mach number, Minf, will be taken as statistically independent random variables. The CFD output is the lift coefficient, Cl.

Traditional Monte Carlo Method

Two independent MC simulations with a sample size of N = 2500 were conducted. In both simulations the average values of the input parameters were set at, $\bar{\mathbf{b}} = \{\bar{\alpha}, \overline{M}\text{inf}\}$ = $\{4^{o}, 0.4\}$. In Simulation 1, $\sigma = \sigma_{\alpha} = \sigma_{Minf} = 0.02$ while in Simulation 2 $\sigma = \sigma_{\alpha} = \sigma_{Minf} = 0.04$. The output function mean and variance were calculated for each simulation. Each independent MC simulation of 2500 samples was subdivided into five samples of N=500. This division allowed for further analysis and comparison of MC techniques. For all MC analyses, standard statistical functions from Microsoft ® Excel 2000 were used and the random number generator MZRAN from [5] was used.

Sensitivity Derivative Enhanced Monte Carlo Method (SDEMC)
Equation 3 was applied to each of the five sub-samples in MC Simulation 1 and in MC Simulation 2. The first-order SD were evaluated once for each sample at the mean values $\overline{\alpha}$ and $\overline{M}inf$. The SD was incorporated in Eq (3) in order to approximate $\overline{C}l$.

Approximate Statistical Moment Method
First and second-order SD were evaluated at the mean values $\overline{\alpha}$ and $\overline{M}inf$ in order to predict $\overline{C}l$ and σ^2_{Cl} as given in (6) and (7). Note that the predictions of $\overline{C}l$ and σ^2_{Cl} are direct calculations and require only one run of the CFD analysis and SD analysis codes.

Sample Results & Discussion

Predictions of $\overline{C}l$ generated via SDEMC methods, as well as $\overline{C}l$ and σ^2_{Cl} generated via approximate statistical moment methods are compared to traditional MC techniques. Before making assessments it is useful to consider the degree of non-linearity in the CFD output function of interest. If the CFD output function, Cl, is quasi-linear with respect to the input variables of interest, one can expect first-order approximations to be reasonably good; that is, the FO moments given by Eq. (6) should match well with the moments produced by a MC simulation. For a nonlinear function, one would expect that uncertainty analyses which include SO terms would yield a better prediction of the statistical moments. In the present analysis one sees nonlinearities in the output function Cl and accordingly second-order approximations should be the better estimates of the moments. When one deviates far from the nominal mean values, the Taylor series approximations are less accurate and the statistical approximations will tend to loose accuracy. It is also worth noting that although the traditional MC analysis is our basis for comparison in the present study, results generated via traditional MC contain error proportional to $\sigma_{Cl}/\sqrt{N}$ (approx 0.0236% for MC Sim 1 and 0.0477% for MC Sim 2.)

Uncertainty Propagation
As shown in Figs. 1 and 2, mean value approximations were compared to the mean values generated using traditional MC simulations with N=2500. Results from five simulations of traditional MC with N=500, five simulations of SDEMC with N=500, a FOFM approximation and a SOFM approximation are shown. For small input deviations (Fig. 1), the inclusion of SD in the MC simulation greatly improves the accuracy of the simulation while at higher input deviations (Fig.2), the inclusion of SD in the comparisons provides no improvement in the accuracy of the simulation. Note that for small input deviations, an order of magnitude improvement is seen SDEMC prediction of the output mean when compared to traditional MC methods. This order of magnitude improvement in accuracy was suggested in [2] and is validated in the present study. Also note that at small input deviations, the SO mean is a very efficient and accurate approximation. Although at high standard deviations inclusion of SD via SDEMC, FOFM, or SOFM methods offers little, if any improvement in accuracy, there are however significant savings in computational resources in each of these methods.

Accurate prediction of output variance or standard deviation is more difficult with percent differences ranging up to 8% (see Figs 3 and 4). In the present study inclusion of SD in SDEMC prediction of variance was not considered. For the second-order variance predictions, no increased accuracy is generated via inclusion of SO terms. However, note that at large input standard deviations, it is more difficult to accurately approximate the output variance as shown in the scaling of Figs 3 and 4.

Timing Considerations

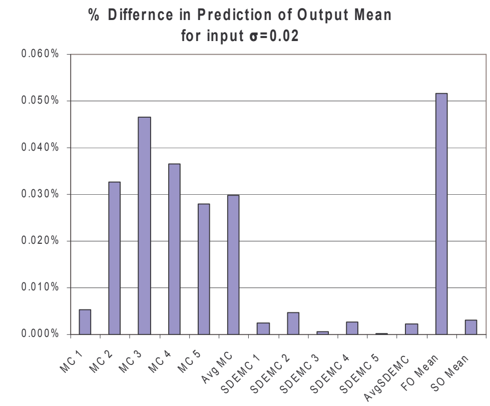
A stochastic analysis with a traditional MC simulation of N runs can be computationally expensive especially when considering CFD codes. In the present study (with two random input variables and one CFD output function), the approximate statistical moment methods are very efficient; the FO method requires approximately the computational equivalent of two analysis runs while the SO method requires approximately the computational equivalent of four analysis runs. Note that the timing associated with each of the FO and SO methods is due to the calculation of first- and second-order SD. With the incremental iterative method used herein, the computational expense is dependent on the number of input variables and output functions. A complete discussion of the dependency is found in [3].

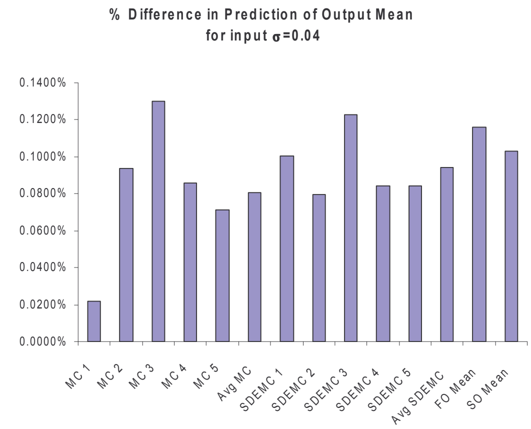
Probability Density Function Approximations

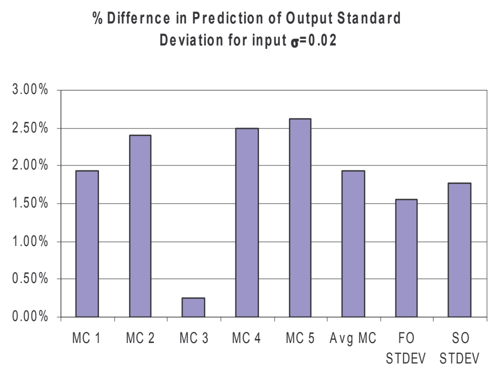
Approximating a mean and standard deviation of the CFD output function and assuming a normal distribution, one may then construct a pdf to approximate the behavior of the non-deterministic output function. This approximation is compared to the pdf histogram generated from a traditional MC simulation in Fig 5 and 6. The bars depict the actual MC simulation histogram, and the solid curve represents the normal distribution at the MC mean value and standard deviation. The MC simulation size of 2500 is not sufficient to obtain a smooth pdf. It is apparent however that for small standard deviations of the input parameters, the normal pdf approximates the actual simulation in regions about the mean but tend to break down in predicting the tails of the distribution. This is significant, for if one is primarily interested in reliable failure predictions, as for structural design, this prediction may not be good enough. It is felt, however, that in aerodynamic performance analysis using CFD, where robustness about the mean is desired, these approximations may suffice.

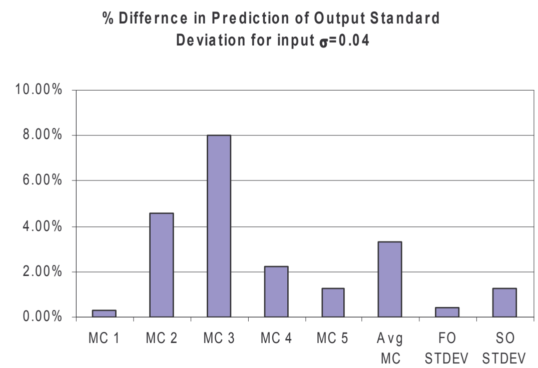
Concluding Remarks and Challenges

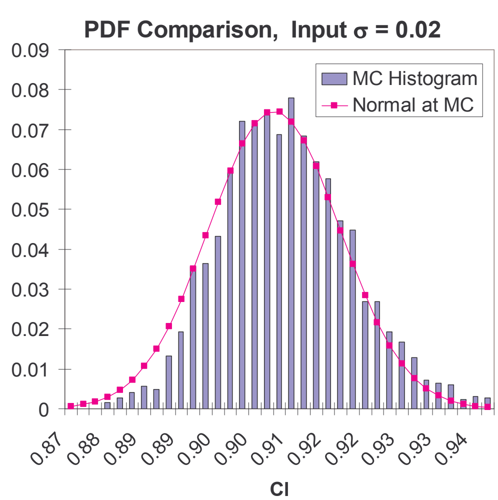
The present results represent an implementation of the SDEMC method and the approximate statistical moment method for uncertainty propagation for 2-D Euler CFD code. Efficient calculation of both first- and second-order sensitivity derivatives was employed and the validity of the approximations was assessed by comparison with statistical moments generated through MC simulations. Collectively, these results demonstrate the possibility for an approach to treat input parameter uncertainty and its propagation through complex CFD analysis without large numbers of samples. The methods are demonstrated on a relatively simple CFD code and problem.

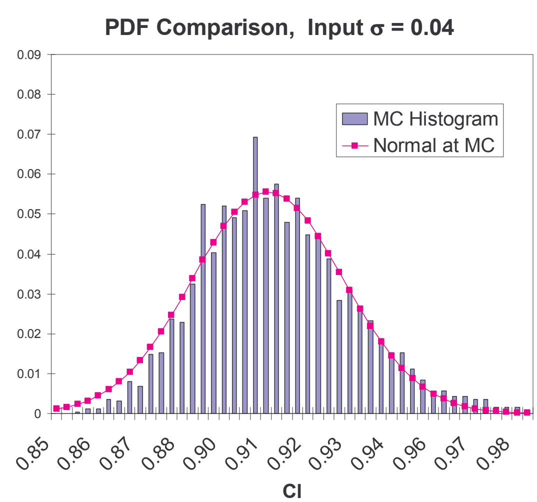












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